Do Spectral Trace Formulæ Converge?

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Abstract

We evaluate the Gutzwiller trace formula for the level density of classically chaotic systems by considering the level density in a bounded energy range and truncating its Fourier integral. This results in a limiting procedure which comprises a convergent semiclassical approximation to a well defined spectral quantity at each stage. We test this result on the spectrum of zeros of the Riemann zeta function, obtaining increasingly good approximations to the level density. The Fourier approach also explains the origin of the convergence problems encountered by the orbit truncation scheme.

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The subject of "quantum chaos" comprises the study of quantum systems whose classical analogue is chaotic. One of the main tools is the Gutzwiller trace formula, which provides a semiclassical approximation (SCA) to the fluctuating part of the quantum level density via an infinite sum over classical periodic orbits. A major problem with this sum is that it does not converge absolutely, making manipulations of the sum rather suspect, and moreover dependent on the ordering.

An important question in this context is whether the Gutzwiller sum can be made to *conditionally* converge, by using an appropriate truncation procedure and possibly a reordering. Convergence in this sense means that one obtains better and better approximations to the level density, limited only by the SCA itself, as the truncation point goes to infinity. The most natural truncation scheme is to include only orbits whose period is bounded by some $T_{\max}$ (we will call this scheme "orbit truncation"). Unfortunately, this has not had much numerical success. Gutzwiller in [1] used orbit truncation to evaluate the semiclassical level density for the anisotropic Kepler problem, and was able to reproduce the level density for low energies but not for higher ones — an incongruous result for an SCA. A mathematical model which is analogous to chaotic systems, the zeros of Riemann's zeta function (see below), displays similar behavior: as one adds "periodic orbits" (prime numbers, in this case) to the sum, peaks in the level density become submerged in increasing oscillations [2]. In the hyperbola billiard there are indications that the sum as written does conditionally converge, however this is an exceptional system in which the Lyapunov exponent is larger than the Kolmogorov entropy [3].

In this work we treat the problem of conditional convergence from a slightly different point of view. We consider $\tilde{d}(\varepsilon)$, the fluctuating part of the level density in a *finite* energy range, and define a purely quantum spectral quantity $\tilde{d}_{\mathcal{T}}(\varepsilon)$ which converges to $\tilde{d}(\varepsilon)$ as $\mathcal{T} \to \infty$. $\tilde{d}_{\mathcal{T}}(\varepsilon)$ is constructed via a smooth truncation of the Fourier transform of $\tilde{d}(\varepsilon)$. We then use the Gutzwiller sum to obtain the SCA to $\tilde{d}_{\mathcal{T}}(\varepsilon)$, which for any $\mathcal{T}$ involves an absolutely converging sum over periodic orbits. The limit $\mathcal{T} \to \infty$ can now be taken safely, avoiding the convergence problems encountered by orbit truncation — the only remaining

errors are due to the SCA itself. This approach differs from previously suggested ones [4–6] in that it does not involve a resummation of the divergent tail of the sum or invoke the bootstrapping mechanism, but rather retains the intuitively appealing ordering by orbit period.

We test this approach ,which we call "Fourier truncation", on the spectrum of zeros of Riemann's zeta function, and obtain very good numerical results. Moreover, we use the Fourier approach to analyze the orbit truncation scheme as well, and show that it leads to incorrect evaluation of the last few "frequency" components of the level density. Because of the exponential proliferation of orbits, these errors can become very large and overwhelm the resulting approximation.

Our starting point is the fluctuating level density $\tilde{d}(E) = \sum_m \delta(E - E_m) - \bar{d}(E)$, where the $\{E_m\}$ are the set of eigenvalues of the Hamiltonian and $\bar{d}(E)$ is the smoothed level density (as given by e.g. Weyl's form). We will confine ourselves to totally hyperbolic time-independent systems with a bounded phase space, in which case the E_m are discrete and correspond to eigenenergies.

We now select a finite energy range $[E_0 \pm \Delta E/2]$ by means of a real and symmetric *window function* $\chi(\varepsilon)$, which satisfies the requirement $\chi(|\varepsilon| > \Delta E/2) \approx 0$. A convenient form is the Gaussian, $\chi(\varepsilon) = \exp(-\varepsilon^2/2\sigma^2)$. We then define the *local* fluctuating part of the level density $\tilde{d}(\varepsilon) = \tilde{d}(E_0 + \varepsilon)\,\chi(\varepsilon)$, and expand it in a Fourier integral,

$$\tilde{d}(\varepsilon) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} d\tau \, \hat{d}(\tau) \exp\left(-i\frac{\tau\varepsilon}{\hbar}\right) , \tag{1a}$$

$$\hat{d}(\tau) = \int_{-\infty}^{\infty} d\varepsilon \, \tilde{d}(\varepsilon) \exp\left(i\frac{\tau\varepsilon}{\hbar}\right) . \tag{1b}$$

The value of $\hat{d}(\tau)$ using the true quantum level density is

$$\hat{d}(\tau) = \sum_m \chi(\varepsilon_m) \exp\left(i\frac{\tau\varepsilon_m}{\hbar}\right) , \tag{2}$$

where $\varepsilon_m = E_m - E_0$. Let us now define $\tilde{d}_{\mathcal{T}}(\varepsilon)$ as the approximation to $\tilde{d}(\varepsilon)$ obtained by truncating $\hat{d}(\tau)$ at $\tau = \mathcal{T}$. We perform this truncation by means of another real and symmetric window function $W_{\mathcal{T}}(\tau)$, which satisfies $W_{\mathcal{T}}(\tau) = 0$ for $|\tau| > \mathcal{T}$. Thus $\tilde{d}(\varepsilon) =$

$\lim_{\mathcal{T}\to\infty}\tilde{d}_{\mathcal{T}}(\varepsilon)$, where

$$\tilde{d}_{\mathcal{T}}(\varepsilon) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} d\tau\, W_{\mathcal{T}}(\tau)\, \hat{d}(\tau)\exp\left(-i\frac{\tau\varepsilon}{\hbar}\right)\ . \tag{3}$$

From (2) $\tilde{d}_{\mathcal{T}}(\varepsilon)$ is given by

$$\tilde{d}_{\mathcal{T}}(\varepsilon) = \sum_m \chi(\varepsilon_m)\, w_{\mathcal{T}}(\varepsilon_m - \varepsilon)\ , \tag{4}$$

where $w_{\mathcal{T}}(\varepsilon) = (2\pi\hbar)^{-1}\int d\tau\, W_{\mathcal{T}}(\tau)\exp(-i\tau\varepsilon/\hbar)$ is the inverse Fourier transform of $W_{\mathcal{T}}(\tau)$. The simplest window one can take is the rectangular or "boxcar" window,

$$W_{\mathcal{T}}^{\mathrm{B}}(\tau) = \begin{cases} 1 & \text{for } |\tau| \leq \mathcal{T}, \\ 0 & \text{otherwise.} \end{cases} \qquad w_{\mathcal{T}}^{\mathrm{B}}(\varepsilon) = 2\mathcal{T}\operatorname{sinc}\left(\frac{\mathcal{T}\varepsilon}{\hbar}\right)\ . \tag{5}$$

$w_{\mathcal{T}}^{\mathrm{B}}(\varepsilon)$ contains long oscillating tails, which fall off asymptotically as $\mathrm{O}(\varepsilon^{-1})$. Since this falloff is only harmonic it may be possible for oscillations from many different delta peaks to interfere coherently to yield large spurious peaks. Thus it may be advisable to choose a different window function.

The problem of estimating the spectrum of an infinite sequence from a finite subset is a common one in signal processing, and a variety of windows, with varying properties, have been developed [7]. One of the more popular is the Hanning window,

$$W_{\mathcal{T}}^{\mathrm{H}}(\tau) = \frac{1}{2}\left[1 + \cos\left(\frac{\pi\tau}{\mathcal{T}}\right)\right]\ , \qquad w_{\mathcal{T}}^{\mathrm{H}}(\varepsilon) = \frac{\pi\sin\left(\frac{\mathcal{T}\varepsilon}{\hbar}\right)}{2\varepsilon\left[\pi^2 - \left(\frac{\mathcal{T}\varepsilon}{\hbar}\right)^2\right]}\ . \tag{6}$$

The largest sidelobe (i.e. tail oscillation) of $w_{\mathcal{T}}^{\mathrm{H}}(\varepsilon)$ is ~ 0.025 the size of the main lobe, vs. ~ 0.22 for the rectangular window. Moreover, the tails of $w_{\mathcal{T}}^{\mathrm{H}}(\varepsilon)$ decay asymptotically as $\mathrm{O}(\varepsilon^{-3})$, and so one need not worry about the cumulative effect of distant tails.

In order to derive the SCA for $\tilde{d}_{\mathcal{T}}(\varepsilon)$ we start from the Gutzwiller sum, which approximates the fluctuating part of the level density by a sum over classical periodic orbits [8],

$$\tilde{d}^{\mathrm{sc}}(E) = \frac{2}{\hbar}\sum_p \sum_{r=1}^{\infty} A_{p,r}(E)\cos\left(\frac{rS_p(E)}{\hbar} - \frac{r\nu_p\pi}{2}\right)\ . \tag{7}$$

Here the summation is over classical primitive periodic orbits p and repetitions r. S_p, T_p, and ν_p are the action, period, and Maslov index of the primitive orbit p, respectively. $A_{p,r}(E) =$

$T_p/|\det(M_p^r - I)|^{1/2}$ is the stability prefactor, where M_p is the monodromy matrix for orbit p. We also restrict the energy range so that E_0 is large enough to be in the semiclassical domain, while ΔE is small enough so that $A_{p,r}(E)$ and $T_p(E)$ can be approximated by their values at E_0, and the action can be replaced by its linearized form, $S_p(E) \approx S_p(E_0) + \varepsilon T_p(E_0)$. In the following quantities without an energy argument refer to their values at E_0.

Next, we insert (7) into (1b) and exchange the order of the p summation and the ε integration. The validity of this step constitutes our primary assumption, and is equivalent to ordering (7) by orbit period. We can then perform the inverse Fourier transform on each term of the sum to get

$$\hat{d}^{\mathrm{sc}}(\tau) = \sum_p \sum_{r=1}^{\infty} A_{p,r} \left\{ \hat{\chi} \left(\frac{\tau + rT_p}{\hbar} \right) \exp\left[ir \left(\frac{S_p}{\hbar} - \frac{\nu_p \pi}{2} \right) \right] \right.$$
$$\left. + \hat{\chi} \left(\frac{\tau - rT_p}{\hbar} \right) \exp\left[-ir \left(\frac{S_p}{\hbar} - \frac{\nu_p \pi}{2} \right) \right] \right\}, \tag{8}$$

where $\hat{\chi}(\tau/\hbar)$ is the Fourier transform of the window function $\chi(\varepsilon)$. For a Gaussian $\chi(\varepsilon)$ it is also a Gaussian, $\hat{\chi}(x) = \sqrt{2\pi\sigma^2} \exp[-(\sigma x)^2/2]$. One can readily verify that (8) is then absolutely convergent, since $\hat{\chi}$ effectively selects for each τ only these orbits (primitive and otherwise) whose period is within a few $\hbar/\sigma$ of τ.

Finally, inserting (8) into (3) and exchanging the summation and integration gives

$$\tilde{d}_{\mathcal{T}}^{\mathrm{sc}}(\varepsilon) = \frac{2}{\hbar} \Re \sum_p \sum_{r=1}^{\infty} A_{p,r}\, \mathcal{F}_{\mathcal{T}}(rT_p, \varepsilon) \exp\left[ir \left(\frac{S_p + \varepsilon T_p}{\hbar} - \frac{\nu_p \pi}{2} \right) \right], \tag{9}$$

where $\mathcal{F}_{\mathcal{T}}(T, \varepsilon)$ is a function which depends on the two windows we used,

$$\mathcal{F}_{\mathcal{T}}(T, \varepsilon) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau\, W_{\mathcal{T}}(\tau + T)\, \hat{\chi}\left(\frac{\tau}{\hbar} \right) \exp\left(-i\frac{\tau\varepsilon}{\hbar} \right). \tag{10}$$

Since $W_{\mathcal{T}}(\tau)$ vanishes for $|\tau| > \mathcal{T}$ and $\hat{\chi}(\tau/\hbar)$ falls off rapidly for $|\tau/\hbar| > \sigma^{-1}$, $\tilde{d}_{\mathcal{T}}^{\mathrm{sc}}(\varepsilon)$ only includes orbits whose period does not extend much beyond $\mathcal{T} + \hbar/\sigma$. Thus for any finite $\mathcal{T}$ one is left with an essentially finite sum, which gives the SCA for the well defined quantum mechanical quantity $\tilde{d}_{\mathcal{T}}(\varepsilon)$. In contrast, an orbit-truncated Gutzwiller sum is not in itself an SCA to anything.

Another way of defining the difference between the two truncation schemes is the following. Suppose that the action is exactly linear in the energy (this is the case for e.g. the wavenumber level density for billiards). Then, approximating the whole spectrum using orbit-truncation corresponds to first taking $\sigma \to \infty$ in (9), and then $\mathcal{T} \to \infty$. However, from (9) it is clear that one should first take the $\mathcal{T} \to \infty$ limit to get the local spectrum, and only then extend to the whole real axis by taking the $\sigma \to \infty$ limit. Since the energy and time to infinity limits do not in general commute, the two truncation schemes can give differing results.

We now test the Fourier truncation method for a particular model, the zeros of the Riemann zeta function on the critical line $z = \frac{1}{2} - iE$. This is a mathematical, rather than a physical, model. However, it is well known that these zeros behave outwardly like the eigenvalues of a chaotic system without any symmetries (see e.g. [2]). Moreover, the fluctuating "level" density for the Riemann zeros on the critical line is exactly given by

$$\tilde{d}(E) = -2 \sum_p \sum_{r=1}^{\infty} \frac{\log p}{2\pi \sqrt{p^r}} \cos(rE \log p) \; , \tag{11}$$

where the p are the prime numbers. Eq. (11) closely resembles the Gutzwiller trace formula (7), with $\hbar = 1$, $\nu_p = 0$, $T_p = \log p$, $S_p = E \log p$, and $A_{p,r} = -\log p / 2\pi \sqrt{p^r}$ (note that here the action is exactly linear in the energy). This "system" is often used in numerical investigations of the properties of various spectral sums, since it is a simple matter to generate millions of prime numbers, while finding periodic orbits in real dynamical systems is a laborious process at best.

Using (11) the equivalent expressions to (8) and (9) for the Riemann zeros are

$$\hat{d}(\tau) = -\sum_p \sum_{r=1}^{\infty} \frac{\log p}{2\pi \sqrt{p^r}} \left\{ \hat{\chi}(\tau + r \log p) \, e^{irE_0 \log p} + \hat{\chi}(\tau - r \log p) \, e^{-irE_0 \log p} \right\} \tag{12a}$$

$$\tilde{d}_{\mathcal{T}}(\varepsilon) = -2 \, \Re \sum_p \sum_{r=1}^{\infty} \frac{\log p}{2\pi \sqrt{p^r}} \, \mathcal{F}_{\mathcal{T}}(r \log p, \, \varepsilon) \, e^{irE \log p} \; . \tag{12b}$$

We test these expressions numerically in Fig. 1. We used 1000, 10,000, 100,000 and 5,761,456 primes (i.e. all primes below 10^8), taking $E_0 = 69.5$ (for historical reasons) and a Gaussian

$\chi(\varepsilon)$ with $\sigma = 2.5$. $\mathcal{T}$ was chosen in each case so that all the Fourier elements considered could be evaluated to a good accuracy using the available primes (more about this later).

The top 4 lines in Fig. 1 show the resulting approximate level density using a rectangular window $W^{\mathrm{B}}_{\mathcal{T}}(\tau)$. We clearly see the δ peaks build up as $\mathcal{T}$ increases. As expected from (4), the amplitude of the intervening oscillations is not strongly dependent on $\mathcal{T}$, but is more or less fixed by the form of $W_{\mathcal{T}}(\tau)$. This is also evident in the bottom 4 lines, where we show the approximate level density using $W^{\mathrm{H}}_{\mathcal{T}}(\tau)$. Here the oscillations are much smaller, at the price of an increase in the width of the peaks, as expected. We conclude that Fourier truncation appears to work very well for the Riemann zeros.

It is instructive to compare Fig. 1 to the level density obtained by orbit truncation at the same place. In this case, as more primes are added to the sum peaks start to emerge, but are eventually obscured by increasing oscillations [2]. We can now understand this behavior by examining Fig. 2, where we show the Fourier spectrum of the truncated sum (11) using the same primes as in Fig. 1. It is apparent that, as more primes are added, a spectral peak builds up near $\tau \approx T_{\mathrm{max}} = \log p_{\mathrm{max}}$ (denoted by a dashed vertical line), where p_{max} is the largest available prime. This peak eventually dominates the resulting level density.

We can understand this peak in the following manner. For large positive $\tau = T_{\mathrm{max}}$ we can approximate (12a) by its second term, and also neglect all repetitions. We can then write $\hat{d}_{T_{\mathrm{max}}}(T_{\mathrm{max}})$ in the presence of orbit truncation in the form of another Fourier transform between the variables x and $\mathcal{E}$, taken at $\mathcal{E} = E_0$,

$$
\hat{d}_{T_{\mathrm{max}}}(T_{\mathrm{max}}, E_0) \approx -\frac{e^{-iE_0 T_{\mathrm{max}}}}{2\pi} \int dx \, \mu(x + T_{\mathrm{max}}) \, \hat{\chi}(x) \, \Theta(-x) e^{-i\mathcal{E}x} \Big|_{\mathcal{E}=E_0}
$$
$$
= \left[\hat{d}(T_{\mathrm{max}}, \mathcal{E}) \otimes \hat{\Theta}^*(\mathcal{E}) \right]_{\mathcal{E}=E_0} , \tag{13}
$$

where $\Theta(x)$ is the step function, $\hat{\Theta}(\mathcal{E}) = \frac{1}{2}\delta(\mathcal{E}) - i/2\pi\mathcal{E}$ is its Fourier transform, $\mu(x)$ is the weighted period density $\mu(x) = \sum_p x \, e^{-\frac{1}{2}x} \, \delta(x - \log p)$, and $\otimes$ denotes a convolution between quantities which are considered functions of $\mathcal{E}$. Since $\hat{\Theta}(\mathcal{E})$ contains long harmonic tails, $\hat{d}_{T_{\mathrm{max}}}(T_{\mathrm{max}})$ will also include $(2\pi E_0)^{-1}$ times the DC ($\mathcal{E} = 0$) component of $\hat{d}(T_{\mathrm{max}})$. From the prime number theorem $\mu(x) \sim \exp(x/2)$, and so for large enough T_{max} we get

$$\left| \hat{d}_{T_{\max}}(T_{\max}) \right| \approx \frac{1}{(2\pi)^2 E_0} \int dx \ \mu(x + T_{\max}) \ \hat{\chi}(x) \approx \frac{e^{1/8\sigma^2}}{2\pi E_0} \ \exp\left(\frac{T_{\max}}{2} \right) \ . \tag{14}$$

Thus the discontinuous truncation "folds" into $\hat{d}_{T_{\max}}(T_{\max})$ an exponentially increasing contribution from the DC component, giving rise to the peak in Fig. 2. The inset of Fig. 2a shows $\hat{d}_{T_{\max}}(T_{\max})$ vs. (14), and we see that the above prediction works quite well.

Finally, we note that unlike in the Riemann case, typical dynamical systems also include Maslov phases. This changes the picture completely, as the DC term which is responsible for the divergent oscillations is then strongly suppressed. We therefore expect that the errors induced by the orbit truncation procedure would in such cases be less severe.

In this work we proposed writing the SCA to the level density of a classically chaotic system by means of a limiting process, consisting at each stage of a convergent SCA to a well defined spectral quantity which itself converges to the level density in the limit. Numerical tests on the application of this method to the Riemann zeros yielded increasingly good approximations to the level density with no divergent oscillations. Moreover, we were able to understand the oscillations that appear in the conventional truncation approach as an edge effect resulting from the abrupt nature of the truncation.

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FIGURES

FIG. 1.   The level density computed using Fourier truncation, using (from bottom to top) 1000, 10,000, 100,000 and 5,761,456 primes. Top 4 lines: Truncating using a rectangular ("boxcar") window. Bottom 4 lines: Truncating using a Hanning window. Each line is shifted upwards by 2 relative to the preceding one. The dashed lines indicate the location of the true Riemann zeros.

FIG. 2.   The Fourier spectrum of the orbit-truncated sum (11), using 1000, 10,000, 100,000 and 5,761,456 primes in subfigures a–d, respectively. The point $\tau = T_{\max}$ is marked by a vertical dashed line. Inset — $|\hat{d}_{T_{\max}}(T_{\max})|$ vs. $T_{\max}$. The dashed line is the prediction of (14).
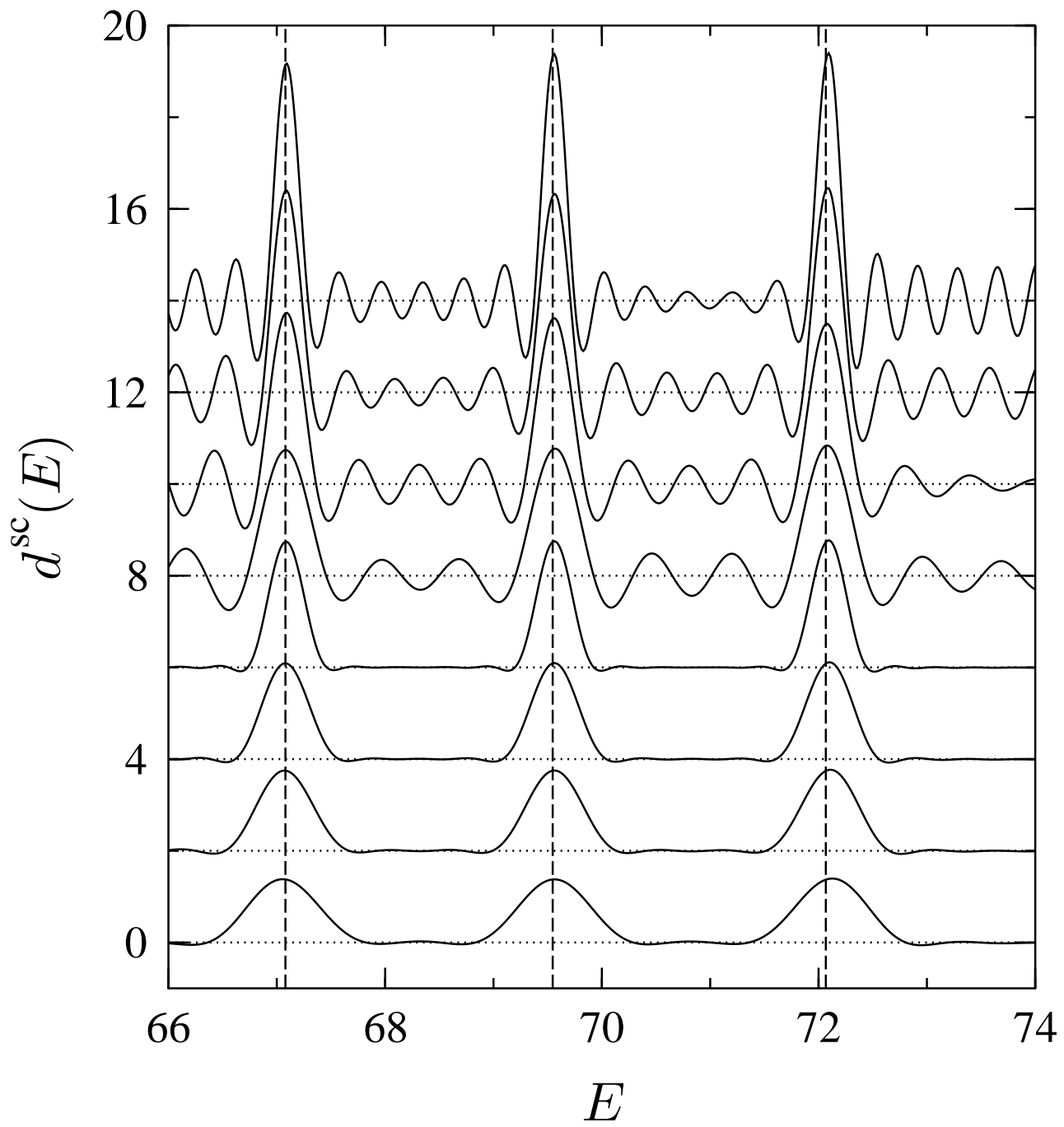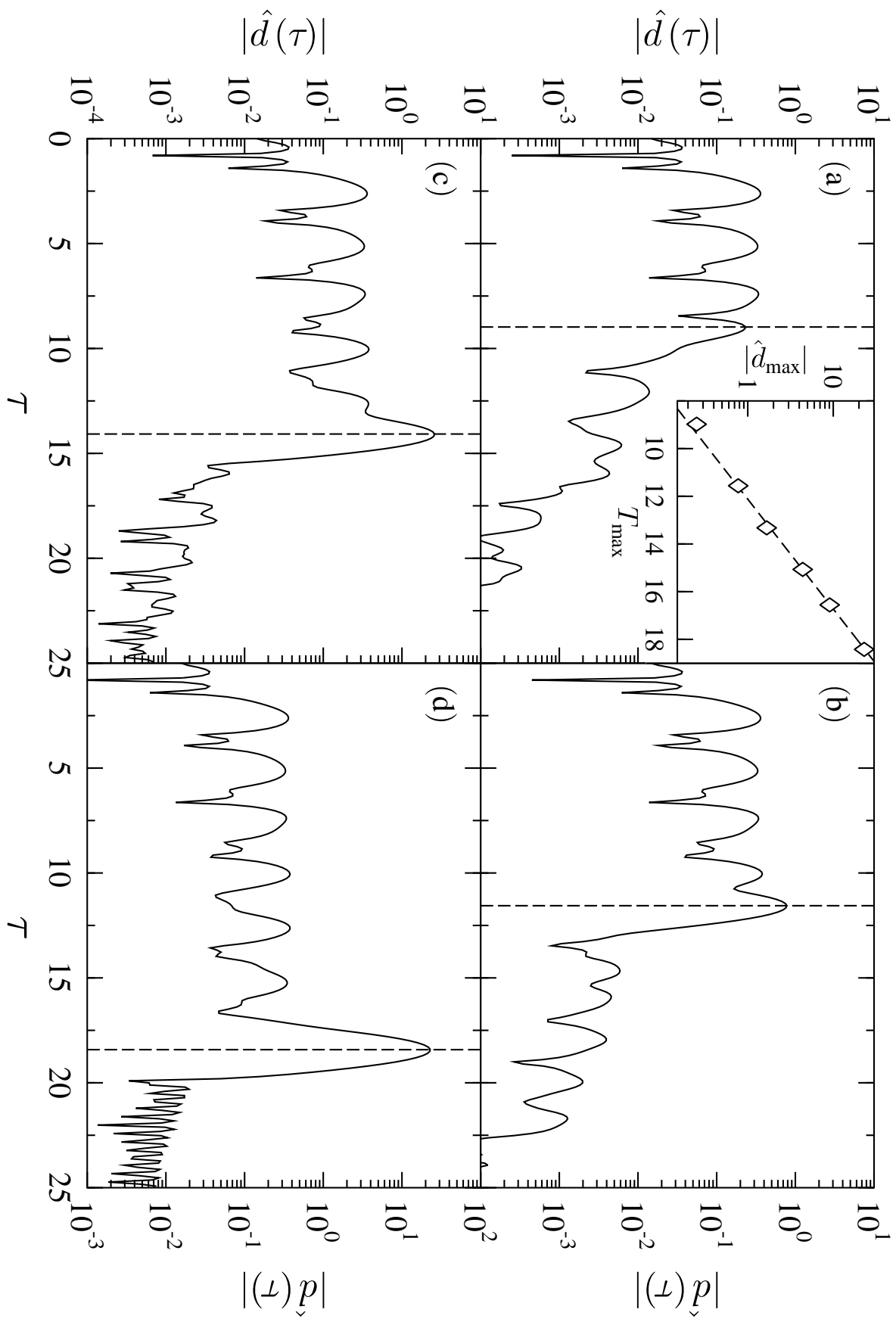
Fig. 1

Fig. 2